Table 1. Crystal data and structure refinement for {CH2(C5H4)2}ZrCl2.

Identification code	ch2s10
Empirical formula	$C_{11}H_{10}Cl_2Zr$
Formula weight	304.31
Temperature	233(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 12.2924(10) Å alpha = 90° b = 11.1466(9) Å beta = 111.1100(10)° c = 8.6500(7) Å gamma = 90°
Volume, Z	1105.67(16) $Å^3$, 4
Density (calculated)	1.828 Mg/m^3
Absorption coefficient	1.432 mm^{-1}
F(000)	600
Crystal size	0.40 x 0.20 x 0.20 mm
θ range for data collection	2.55 to 28.04°
Limiting indices	$-16 \le h \le 15$, $-14 \le k \le 13$, $-7 \le l \le 11$
Reflections collected	3708
Independent reflections	1254 (R_{int} = 0.0174)
Completeness to θ = 28.04°	93.4 %
Absorption correction	SADABS
Max. and min. transmission	0.7627 and 0.5981
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1254 / 0 / 66
Goodness-of-fit on F^2	1.090
Final R indices [I>2σ(I)]	R1 = 0.0188, wR2 = 0.0503
R indices (all data)	R1 = 0.0197, wR2 = 0.0508
Extinction coefficient	0.0020(4)
Largest diff. peak and hole	0.258 and -0.274 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for {CH2(C5H4)2}ZrCl2. U(eq) is de one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr	0	1935(1)	2500	32(1)
Cl	-1548(1)	510(1)	1087(1)	51(1)
C(1)	0	4728(2)	2500	55(1)
C(11)	311(2)	3860(2)	1363(2)	46(1)
C(12)	1380(2)	3249(2)	1799(3)	48(1)
C(13)	1228(2)	2263(2)	705(3)	50(1)
C(14)	71(2)	2241(2)	-365(2)	50(1)
C(15)	-512(2)	3221(2)	48(2)	48(1)

Table 3. Bond lengths [Å] and angles [°] for {CH2(C5H4)2}ZrCl2.

Zr-Cl	2.4416(5)	Zr-Cl#1	2.4416(5)
Zr-C(15)#1	2.4472(18)	Zr-C(15)	2.4472(18)
Zr-C(11)	2.4478(16)	Zr-C(11)#1	2.4478(16)
Zr-C(12)	2.4766(18)	Zr-C(12)#1	2.4766(18)
Zr-C(14)	2.5337(17)	Zr-C(14)#1	2.5337(17)
Zr-C(13)	2.5512(17)	Zr-C(13)#1	2.5512(17)
C(1)-C(11)	1.523(2)	C(1)-C(11)#1	1.523(2)
C(11)-C(12)	1.406(3)	C(11)-C(15)	1.413(3)
C(12)-C(13)	1.418(3)	C(13)-C(14)	1.390(3)
C(14)-C(15)	1.420(3)		
Cl-Zr-Cl#1	98.84(2)	Cl-Zr-C(15)#1	136.53(5)
Cl#1-Zr-C(15)#1	92.08(5)	Cl-Zr-C(15)	92.08(5)
Cl#1-Zr-C(15)	136.53(5)	C(15)#1-Zr-C(15)	108.28(9)
Cl-Zr-C(11)	125.14(5)	Cl#1-Zr-C(11)	124.41(5)
C(15)#1-Zr-C(11)	78.81(6)	C(15)-Zr-C(11)	33.56(7)
Cl-Zr-C(11)#1	124.41(5)	Cl#1-Zr-C(11)#1	125.14(5)
C(15)#1-Zr-C(11)#1	33.56(7)	C(15)-Zr-C(11)#1	78.81(6)
C(11)-Zr-C(11)#1	57.47(8)	Cl-Zr-C(12)	137.83(5)
Cl#1-Zr-C(12)	91.62(5)	C(15)#1-Zr-C(12)	83.15(7)
C(15)-Zr-C(12)	55.00(7)	C(11)-Zr-C(12)	33.18(7)
C(11)#1-Zr-C(12)	78.46(6)	Cl-Zr-C(12)#1	91.62(5)
Cl#1-Zr-C(12)#1	137.83(5)	C(15)#1-Zr-C(12)#1	54.99(7)
C(15)-Zr-C(12)#1	83.15(7)	C(11)-Zr-C(12)#1	78.46(6)
C(11)#1-Zr-C(12)#1	33.18(7)	C(12)-Zr-C(12)#1	107.49(9)
Cl-Zr-C(14)	83.86(5)	Cl#1-Zr-C(14)	106.40(5)
C(15)#1-Zr-C(14)	132.85(7)	C(15)-Zr-C(14)	33.08(6)
C(11)-Zr-C(14)	54.80(6)	C(11)#1-Zr-C(14)	109.89(6)
C(12)-Zr-C(14)	54.06(7)	C(12)#1-Zr-C(14)	115.32(7)
Cl-Zr-C(14)#1	106.40(5)	Cl#1-Zr-C(14)#1	83.86(5)
C(15)#1-Zr-C(14)#1	33.08(6)	C(15)-Zr-C(14)#1	132.85(7)
C(11)-Zr-C(14)#1	109.89(6)	C(11)#1-Zr-C(14)#1	54.80(6)
C(12)-Zr-C(14)#1	115.32(7)	C(12)#1-Zr-C(14)#1	54.06(7)
C(14)-Zr-C(14)#1	164.51(9)	Cl-Zr-C(13)	108.28(5)
Cl#1-Zr-C(13)	82.69(5)	C(15)#1-Zr-C(13)	114.81(7)
C(15)-Zr-C(13)	54.02(7)	C(11)-Zr-C(13)	54.38(6)
C(11)#1-Zr-C(13)	109.34(6)	C(12)-Zr-C(13)	32.72(6)
C(12)#1-Zr-C(13)	132.21(7)	C(14)-Zr-C(13)	31.73(7)
C(14)#1-Zr-C(13)	144.29(7)	Cl-Zr-C(13)#1	82.69(5)
Cl#1-Zr-C(13)#1	108.28(5)	C(15)#1-Zr-C(13)#1	54.02(7)
C(15)-Zr-C(13)#1	114.81(7)	C(11)-Zr-C(13)#1	109.34(6)
C(11)#1-Zr-C(13)#1	54.38(6)	C(12)-Zr-C(13)#1	132.21(7)
C(12)#1-Zr-C(13)#1	32.72(6)	C(14)-Zr-C(13)#1	144.29(7)
C(14)#1-Zr-C(13)#1	31.73(7)	C(13)-Zr-C(13)#1	163.53(9)
C(11)-C(1)-C(11)#1	101.18(19)	C(12)-C(11)-C(15)	107.49(16)
C(12)-C(11)-C(1)	124.23(16)	C(15)-C(11)-C(1)	124.49(17)
C(12)-C(11)-Zr	74.54(10)	C(15)-C(11)-Zr	73.20(10)
C(1)-C(11)-Zr	100.67(11)	C(11)-C(12)-C(13)	108.10(18)
C(11)-C(12)-Zr	72.29(10)	C(13)-C(12)-Zr	76.54(10)
C(14)-C(13)-C(12)	108.39(18)	C(14)-C(13)-Zr	73.44(10)
C(12)-C(13)-Zr	70.75(10)	C(13)-C(14)-C(15)	107.88(17)
C(13)-C(14)-Zr	74.83(10)	C(15)-C(14)-Zr	70.12(10)
C(11)-C(15)-C(14)	108.08(19)	C(11)-C(15)-Zr	73.24(10)
C(14)-C(15)-Zr	76.81(10)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for {CH2(C5H4)2}ZrCl2.

The anisotropic displacement factor exponent takes the f $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Zr	43(1)	24(1)	33(1)	0	18(1)	0
Cl	50(1)	38(1)	60(1)	-9(1)	15(1)	-7(1)
C(1)	95(2)	26(1)	63(2)	0	49(2)	0
C(11)	75(1)	28(1)	47(1)	6(1)	38(1)	-1(1)
C(12)	61(1)	38(1)	56(1)	-1(1)	36(1)	-10(1)
C(13)	67(1)	40(1)	60(1)	-1(1)	45(1)	0(1)
C(14)	78(1)	43(1)	37(1)	-1(1)	32(1)	-2(1)
C(15)	70(1)	40(1)	40(1)	10(1)	27(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for {CH2(C5H4)2}ZrCl2.

	x	y	z	U(eq)
H(1A)	-664	5236	1880	66
H(1B)	664	5236	3120	66
H(12A)	2137	3540	2590	57
H(13A)	1854	1725	649	60
H(14A)	-265	1697	-1324	59
H(15A)	-1308	3501	-616	58

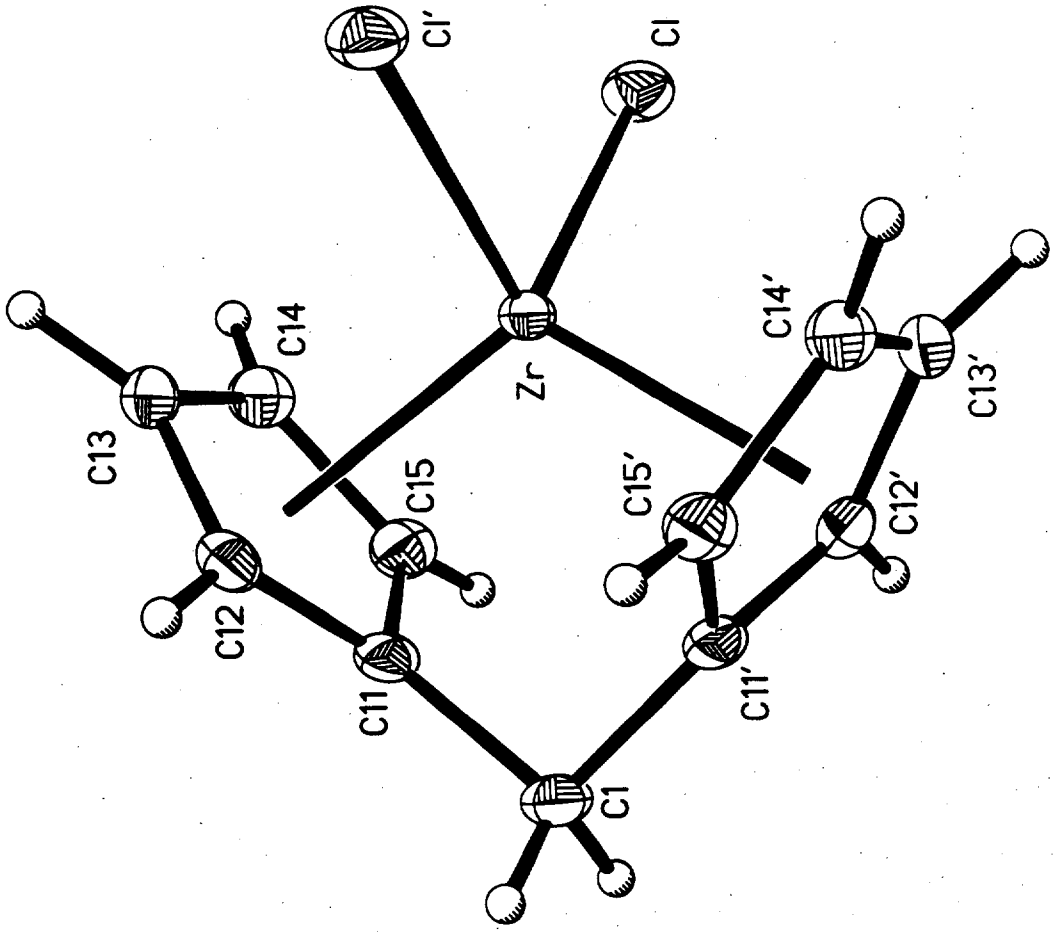
Cl'
Cl
Zr
C14
C13
C15
C12
C11
C1
C14'
C13'
C15'
C12'
C11'

Table 1. Crystal data and structure refinement for [CH2(C5H4)2]ZrI2.

Identification code	ds10
Empirical formula	$C_{11}H_{10}I_2Zr$
Formula weight	487.21
Temperature	233(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Cmcm
Unit cell dimensions	a = 12.4688(13) Å alpha = 90° b = 11.4786(11) Å beta = 90° c = 8.6910(9) Å gamma = 90°
Volume, Z	1243.9(2) $Å^3$, 4
Density (calculated)	2.602 Mg/m^3
Absorption coefficient	5.808 mm^{-1}
F(000)	888
Crystal size	0.50 x 0.50 x 0.30 mm
θ range for data collection	2.41 to 28.19°
Limiting indices	$-15 \le h \le 14$, $-15 \le k \le 11$, $-11 \le l \le 10$
Reflections collected	4139
Independent reflections	798 (R_{int} = 0.0236)
Completeness to θ = 28.19°	93.4 %
Absorption correction	SADABS
Max. and min. transmission	0.2747 and 0.1593
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	798 / 0 / 43
Goodness-of-fit on F^2	1.135
Final R indices [I>2σ(I)]	R1 = 0.0248, wR2 = 0.0570
R indices (all data)	R1 = 0.0261, wR2 = 0.0577
Extinction coefficient	0.00244(18)

Largest diff. peak and hole	0.835 and -0.818 eÅ

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [CH2(C5H4)2]ZrI2. U(eq) is def one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr	0	2112(1)	2500	23(1)
I	1767(1)	579(1)	2500	43(1)
C(11)	0	3975(4)	1154(5)	31(1)
C(12)	915(3)	3368(3)	620(4)	36(1)
C(13)	557(3)	2421(3)	-291(4)	42(1)
C(21)	0	4817(6)	2500	34(2)

Table 3. Bond lengths [Å] and angles [°] for [CH2(C5H4)2]ZrI2.

Zr-C(11)#1	2.438(4)	Zr-C(11)	2.438(4)
Zr-C(12)#1	2.460(3)	Zr-C(12)#2	2.460(3)
Zr-C(12)#3	2.460(3)	Zr-C(12)	2.460(3)
Zr-C(13)#2	2.548(3)	Zr-C(13)	2.548(3)
Zr-C(13)#1	2.548(3)	Zr-C(13)#3	2.548(3)
Zr-I#3	2.8188(5)	Zr-I	2.8188(5)
C(11)-C(12)#2	1.415(4)	C(11)-C(12)	1.415(4)
C(11)-C(21)	1.517(6)	C(12)-C(13)	1.417(5)
C(13)-C(13)#2	1.388(8)	C(21)-C(11)#1	1.517(6)

C(11)#1-Zr-C(11)	57.3(2)	C(11)#1-Zr-C(12)#1	33.59(10)
C(11)-Zr-C(12)#1	78.72(13)	C(11)#1-Zr-C(12)#2	78.72(13)
C(11)-Zr-C(12)#2	33.59(10)	C(12)#1-Zr-C(12)#2	108.23(17)
C(11)#1-Zr-C(12)#3	33.59(10)	C(11)-Zr-C(12)#3	78.72(13)
C(12)#1-Zr-C(12)#3	55.24(18)	C(12)#2-Zr-C(12)#3	83.27(18)
C(11)#1-Zr-C(12)	78.72(13)	C(11)-Zr-C(12)	33.59(10)
C(12)#1-Zr-C(12)	83.27(18)	C(12)#2-Zr-C(12)	55.24(18)
C(12)#3-Zr-C(12)	108.23(17)	C(11)#1-Zr-C(13)#2	109.54(14)
C(11)-Zr-C(13)#2	54.63(13)	C(12)#1-Zr-C(13)#2	132.63(13)
C(12)#2-Zr-C(13)#2	32.81(12)	C(12)#3-Zr-C(13)#2	115.13(13)
C(12)-Zr-C(13)#2	53.99(12)	C(11)#1-Zr-C(13)	109.54(14)
C(11)-Zr-C(13)	54.63(13)	C(12)#1-Zr-C(13)	115.13(13)
C(12)#2-Zr-C(13)	53.99(12)	C(12)#3-Zr-C(13)	132.63(13)
C(12)-Zr-C(13)	32.81(12)	C(13)#2-Zr-C(13)	31.61(18)
C(11)#1-Zr-C(13)#1	54.63(13)	C(11)-Zr-C(13)#1	109.54(14)
C(12)#1-Zr-C(13)#1	32.81(12)	C(12)#2-Zr-C(13)#1	132.63(13)
C(12)#3-Zr-C(13)#1	53.99(12)	C(12)-Zr-C(13)#1	115.13(13)
C(13)#2-Zr-C(13)#1	163.99(17)	C(13)-Zr-C(13)#1	144.37(19)
C(11)#1-Zr-C(13)#3	54.63(13)	C(11)-Zr-C(13)#3	109.54(14)
C(12)#1-Zr-C(13)#3	53.99(12)	C(12)#2-Zr-C(13)#3	115.13(13)
C(12)#3-Zr-C(13)#3	32.81(12)	C(12)-Zr-C(13)#3	132.63(13)
C(13)#2-Zr-C(13)#3	144.37(19)	C(13)-Zr-C(13)#3	163.99(17)
C(13)#1-Zr-C(13)#3	31.61(19)	C(11)#1-Zr-I#3	123.19(4)
C(11)-Zr-I#3	123.19(4)	C(12)#1-Zr-I#3	136.72(9)
C(12)#2-Zr-I#3	90.20(9)	C(12)#3-Zr-I#3	90.20(9)
C(12)-Zr-I#3	136.72(9)	C(13)#2-Zr-I#3	82.76(9)
C(13)-Zr-I#3	107.44(9)	C(13)#1-Zr-I#3	107.44(9)
C(13)#3-Zr-I#3	82.76(9)	C(11)#1-Zr-I	123.19(4)
C(11)-Zr-I	123.19(4)	C(12)#1-Zr-I	90.20(9)
C(12)#2-Zr-I	136.72(9)	C(12)#3-Zr-I	136.72(9)
C(12)-Zr-I	90.20(9)	C(13)#2-Zr-I	107.44(9)
C(13)-Zr-I	82.76(9)	C(13)#1-Zr-I	82.76(9)
C(13)#3-Zr-I	107.44(9)	I#3-Zr-I	102.79(3)
C(12)#2-C(11)-C(12)	107.4(4)	C(12)#2-C(11)-C(21)	124.5(2)
C(12)-C(11)-C(21)	124.5(2)	C(12)#2-C(11)-Zr	74.1(2)
C(12)-C(11)-Zr	74.1(2)	C(21)-C(11)-Zr	100.9(3)
C(11)-C(12)-C(13)	107.9(3)	C(11)-C(12)-Zr	72.4(2)
C(13)-C(12)-Zr	77.0(2)	C(13)#2-C(13)-C(12)	108.4(2)
C(13)#2-C(13)-Zr	74.19(9)	C(12)-C(13)-Zr	70.18(19)
C(11)-C(21)-C(11)#1	100.9(5)		

Symmetry transformations used to generate equivalent atoms:

#1 x,y,-z+1/2 #2 -x,y,z #3 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for [CH2(C5H4)2]ZrI2.

The anisotropic displacement factor exponent takes the fo $-2\pi^2$ [$(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}$]

	U11	U22	U33	U23	U13	U12
Zr	27(1)	20(1)	22(1)	0	0	0
I	39(1)	41(1)	50(1)	0	0	15(1)
C(11)	43(3)	22(2)	27(2)	6(2)	0	0
C(12)	40(2)	36(2)	33(2)	8(1)	9(2)	-3(2)
C(13)	64(2)	37(2)	25(2)	2(1)	11(2)	7(2)
C(21)	44(4)	25(3)	34(3)	0	0	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [CH2(C5H4)2]ZrI2.

	x	y	z	U(eq)
H(12A)	1665	3644	696	43
H(13A)	1020	1894	-901	50
H(21)	-590(40)	5270(50)	2500	28(13)

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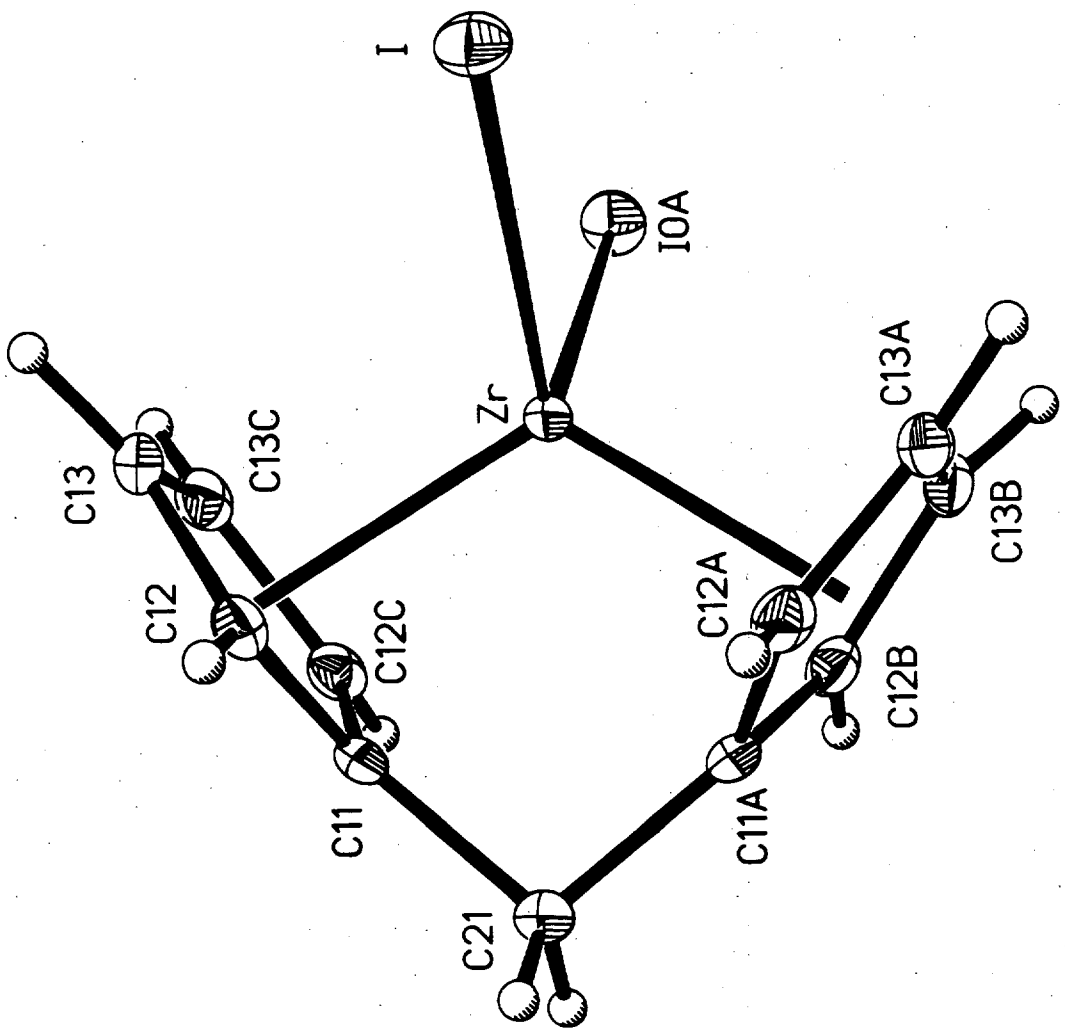

Table 1. Crystal data and structure refinement for (CHCp)2ZrCl2.

Identification code	jj10
Empirical formula	$C_{12}H_{12}Cl_2Zr$
Formula weight	318.34
Temperature	233(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 13.411(12) Å alpha = 90° b = 8.227(7) Å beta = 119.862(13)° c = 12.280(11) Å gamma = 90°
Volume, Z	1174.9(18) $Å^3$, 4
Density (calculated)	1.800 Mg/m^3
Absorption coefficient	1.352 mm^{-1}
F(000)	632
Crystal size	0.20 x 0.20 x 0.10 mm
θ range for data collection	3.03 to 28.34°
Limiting indices	$-15 \le h \le 17$, $-5 \le k \le 10$, $-15 \le l \le 12$
Reflections collected	2860
Independent reflections	1328 (R_{int} = 0.0283)
Completeness to θ = 28.34°	90.2 %
Absorption correction	SADABS
Max. and min. transmission	0.8766 and 0.7737
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1328 / 13 / 125
Goodness-of-fit on F^2	1.026
Final R indices [I>2σ(I)]	R1 = 0.0283, wR2 = 0.0730
R indices (all data)	R1 = 0.0303, wR2 = 0.0742
Extinction coefficient	0.0000(4)
Largest diff. peak and hole	0.627 and -0.661 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for (CHCp)2ZrCl2. U(eq) is defined one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr	0	4485(1)	2500	33(1)
Cl	-37(1)	2540(1)	997(1)	67(1)
C(1)	-1220(20)	6979(19)	1963(18)	42(3)
C(2)	-1410(14)	6249(19)	832(12)	45(2)
C(3)	-1998(11)	4782(16)	685(13)	54(2)
C(4)	-2120(9)	4575(11)	1710(15)	57(3)
C(5)	-1603(12)	5883(15)	2539(12)	48(2)
C(6)	-559(5)	8530(8)	2526(10)	46(2)
C(1A)	-1150(30)	6980(30)	1850(20)	43(6)
C(2A)	-1670(20)	5950(30)	786(18)	54(5)
C(3A)	-2143(11)	4638(19)	1070(20)	57(5)
C(4A)	-1948(14)	4840(20)	2260(20)	53(4)
C(5A)	-1336(15)	6260(30)	2768(14)	46(3)
C(6A)	-588(8)	8589(10)	1936(18)	54(3)

Table 3. Bond lengths [Å] and angles [°] for (CHCp)2ZrCl2.

Zr-Cl	2.4244(17)	Zr-Cl#1	2.4244(17)
Zr-C(1)#1	2.50(3)	Zr-C(1)	2.50(3)
Zr-C(2)#1	2.454(16)	Zr-C(2)	2.454(16)
Zr-C(5)#1	2.459(13)	Zr-C(5)	2.459(13)
Zr-C(5A)#1	2.457(19)	Zr-C(5A)	2.457(19)
Zr-C(2A)#1	2.49(3)	Zr-C(2A)	2.49(3)
C(1)-C(5)	1.396(10)	C(1)-C(2)	1.413(11)
C(1)-C(6)	1.508(9)	C(2)-C(3)	1.403(12)
C(3)-C(4)	1.359(11)	C(4)-C(5)	1.404(11)
C(6)-C(6)#1	1.533(14)	C(1A)-C(5A)	1.402(14)
C(1A)-C(2A)	1.411(13)	C(1A)-C(6A)	1.502(12)
C(2A)-C(3A)	1.385(15)	C(3A)-C(4A)	1.357(14)
C(4A)-C(5A)	1.387(14)	C(6A)-C(6A)#1	1.49(2)

Cl-Zr-Cl#1	97.43(8)	Cl-Zr-C(1)#1	120.4(3)
Cl#1-Zr-C(1)#1	125.3(4)	Cl-Zr-C(1)	125.3(4)
Cl#1-Zr-C(1)	120.4(3)	C(1)#1-Zr-C(1)	69.4(8)
Cl-Zr-C(2)#1	137.8(3)	Cl#1-Zr-C(2)#1	92.3(3)
C(1)#1-Zr-C(2)#1	33.1(3)	C(1)-Zr-C(2)#1	82.2(6)
Cl-Zr-C(2)	92.3(3)	Cl#1-Zr-C(2)	137.8(3)
C(1)#1-Zr-C(2)	82.2(6)	C(1)-Zr-C(2)	33.1(3)
C(2)#1-Zr-C(2)	107.5(7)	Cl-Zr-C(5)#1	88.9(3)
Cl#1-Zr-C(5)#1	129.6(3)	C(1)#1-Zr-C(5)#1	32.7(3)
C(1)-Zr-C(5)#1	94.2(5)	C(2)#1-Zr-C(5)#1	54.7(4)
C(2)-Zr-C(5)#1	91.4(4)	Cl-Zr-C(5)	129.6(3)
Cl#1-Zr-C(5)	88.9(3)	C(1)#1-Zr-C(5)	94.2(5)
C(1)-Zr-C(5)	32.7(3)	C(2)#1-Zr-C(5)	91.4(4)
C(2)-Zr-C(5)	54.7(4)	C(5)#1-Zr-C(5)	124.2(5)
Cl-Zr-C(5A)#1	91.7(4)	Cl#1-Zr-C(5A)#1	139.0(4)
C(1)#1-Zr-C(5A)#1	28.8(6)	C(1)-Zr-C(5A)#1	84.3(6)
C(2)#1-Zr-C(5A)#1	56.6(6)	C(2)-Zr-C(5A)#1	81.2(4)
C(5)#1-Zr-C(5A)#1	10.5(3)	C(5)-Zr-C(5A)#1	115.3(6)
Cl-Zr-C(5A)	139.0(4)	Cl#1-Zr-C(5A)	91.7(4)
C(1)#1-Zr-C(5A)	84.3(6)	C(1)-Zr-C(5A)	28.8(6)
C(2)#1-Zr-C(5A)	81.2(4)	C(2)-Zr-C(5A)	56.6(6)
C(5)#1-Zr-C(5A)	115.3(6)	C(5)-Zr-C(5A)	10.5(3)
C(5A)#1-Zr-C(5A)	107.1(9)	Cl-Zr-C(2A)#1	129.2(5)
Cl#1-Zr-C(2A)#1	90.4(5)	C(1)#1-Zr-C(2A)#1	35.4(7)
C(1)-Zr-C(2A)#1	91.0(5)	C(2)#1-Zr-C(2A)#1	9.3(5)
C(2)-Zr-C(2A)#1	114.4(5)	C(5)#1-Zr-C(2A)#1	50.5(6)
C(5)-Zr-C(2A)#1	100.5(4)	C(5A)#1-Zr-C(2A)#1	54.3(5)
C(5A)-Zr-C(2A)#1	90.4(5)	Cl-Zr-C(2A)	90.4(5)
Cl#1-Zr-C(2A)	129.2(5)	C(1)#1-Zr-C(2A)	91.0(5)
C(1)-Zr-C(2A)	35.4(7)	C(2)#1-Zr-C(2A)	114.4(5)
C(2)-Zr-C(2A)	9.3(5)	C(5)#1-Zr-C(2A)	100.5(4)
C(5)-Zr-C(2A)	50.5(6)	C(5A)#1-Zr-C(2A)	90.4(5)
C(5A)-Zr-C(2A)	54.3(5)	C(2A)#1-Zr-C(2A)	122.0(9)
C(5)-C(1)-C(2)	106.9(8)	C(5)-C(1)-C(6)	126.4(11)
C(2)-C(1)-C(6)	126.2(11)	C(5)-C(1)-Zr	72.2(11)
C(2)-C(1)-Zr	71.8(12)	C(6)-C(1)-Zr	114.8(16)
C(3)-C(2)-C(1)	108.0(9)	C(3)-C(2)-Zr	75.4(8)
C(1)-C(2)-Zr	75.1(13)	C(4)-C(3)-C(2)	107.9(10)
C(4)-C(3)-Zr	74.5(8)	C(2)-C(3)-Zr	71.7(9)
C(3)-C(4)-C(5)	109.4(9)	C(3)-C(4)-Zr	74.0(7)
C(5)-C(4)-Zr	71.7(6)	C(4)-C(5)-C(1)	107.6(8)

C(4)-C(5)-Zr	75.5(7)	C(1)-C(5)-Zr	75.1(13)
C(1)-C(6)-C(6)#1	109.9(11)	C(5A)-C(1A)-C(2A)	106.8(10)
C(5A)-C(1A)-C(6A)	126.8(15)	C(2A)-C(1A)-C(6A)	126.3(15)
C(5A)-C(1A)-Zr	73.5(16)	C(2A)-C(1A)-Zr	74.8(18)
C(6A)-C(1A)-Zr	120(2)	C(3A)-C(2A)-C(1A)	108.1(12)
C(3A)-C(2A)-Zr	75.0(12)	C(1A)-C(2A)-Zr	72.0(19)
C(4A)-C(3A)-C(2A)	108.1(12)	C(4A)-C(3A)-Zr	73.4(9)
C(2A)-C(3A)-Zr	72.9(13)	C(3A)-C(4A)-C(5A)	109.9(13)
C(3A)-C(4A)-Zr	75.2(9)	C(5A)-C(4A)-Zr	72.2(10)
C(4A)-C(5A)-C(1A)	107.1(11)	C(4A)-C(5A)-Zr	75.2(10)
C(1A)-C(5A)-Zr	73.3(18)	C(6A)#1-C(6A)-C(1A)	109.3(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for (CHCp)2ZrCl2.

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2 U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Zr	38(1)	24(1)	40(1)	0	21(1)	0
Cl	112(1)	43(1)	64(1)	-10(1)	58(1)	-3(1)
C(1)	37(7)	31(6)	58(6)	-2(4)	24(5)	7(4)
C(2)	38(6)	34(3)	48(4)	7(2)	11(3)	4(3)
C(3)	39(5)	43(4)	62(5)	-6(4)	12(3)	-8(3)
C(4)	42(5)	46(4)	86(11)	-11(8)	34(9)	-13(3)
C(5)	40(6)	44(6)	74(6)	-7(4)	38(5)	-8(4)
C(6)	47(3)	29(2)	63(4)	0(3)	29(3)	6(2)
C(1A)	23(6)	33(9)	70(12)	8(7)	21(8)	2(5)
C(2A)	38(10)	62(14)	50(6)	3(6)	12(5)	12(7)
C(3A)	30(5)	58(9)	71(15)	-18(12)	16(9)	-9(4)
C(4A)	35(6)	53(9)	76(10)	-1(7)	31(7)	-5(5)
C(5A)	30(7)	44(8)	62(6)	-10(5)	21(5)	2(5)
C(6A)	47(4)	25(3)	72(8)	5(4)	17(5)	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (CHCp)2ZrCl2.

	x	y	z	U(eq)
H(2)	-1303	6786	177	54
H(3)	-2352	4097	-80	65
H(4)	-2571	3699	1816	69
H(5)	-1659	6103	3299	58
H(61)	-382	8624	3400	55
H(62)	-1032	9466	2059	55
H(2A)	-1772	6209	-52	65
H(3A)	-2629	3785	473	69
H(4A)	-2275	4140	2660	64
H(5A)	-1191	6772	3563	56
H(61A)	-536	8772	1177	64
H(62A)	-1048	9468	2004	64

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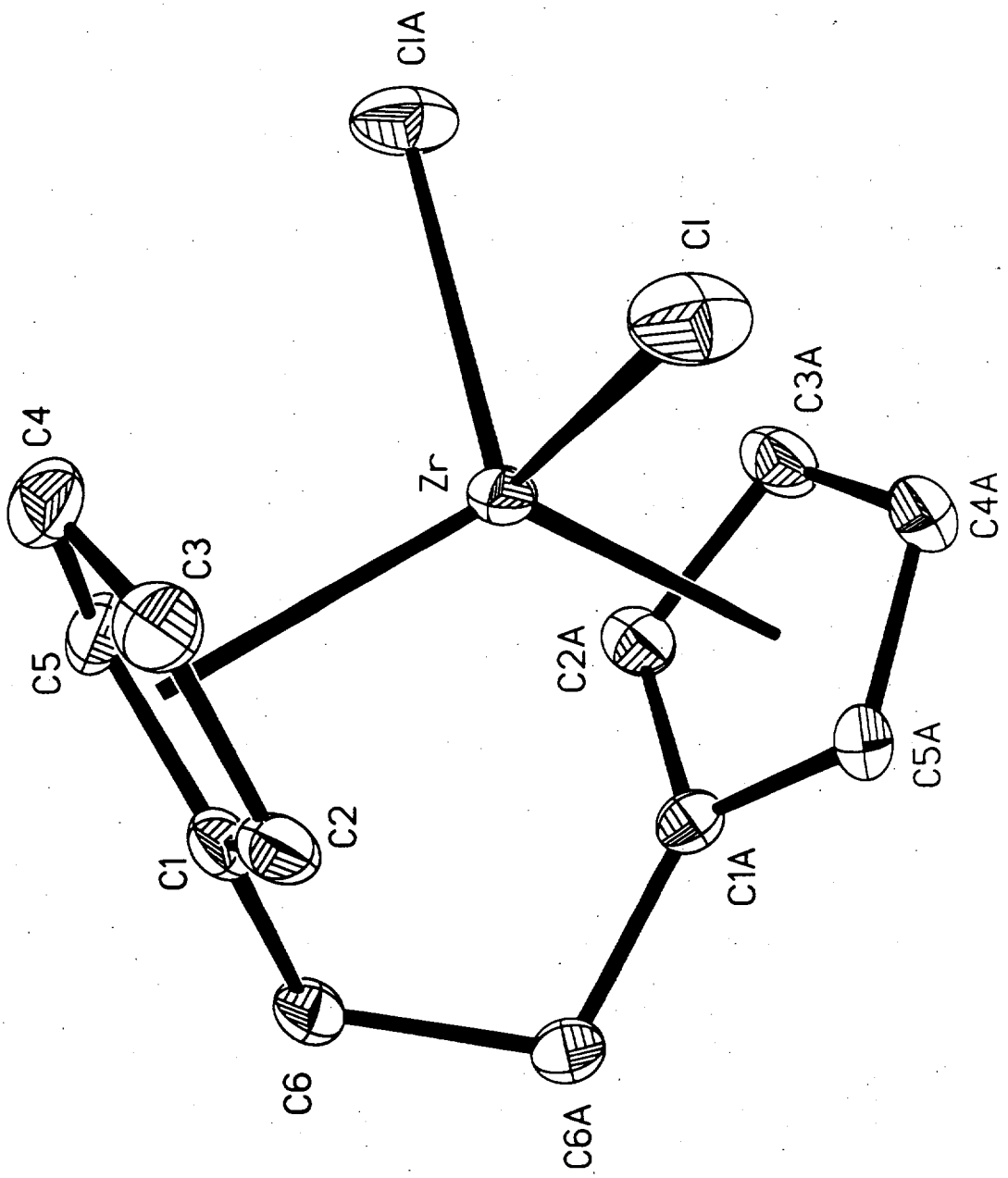

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